

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 30.11.2015

Version 16.14

SECTION 1. Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Catalogue No.	101789
Product name	Benzene-D6 deuteration degree min. 99.6% for NMR spectroscopy MagniSolv™
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	1076-43-3

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses	Reagent for analysis For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com).
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1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number	Please contact the regional company representation in your country.
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SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Flammable liquid, Category 2, H225
Carcinogenicity, Category 1A, H350
Germ cell mutagenicity, Category 1B, H340
Specific target organ toxicity - repeated exposure, Category 1, H372
Aspiration hazard, Category 1, H304
Eye irritation, Category 2, H319
Skin irritation, Category 2, H315

For the full text of the H-Statements mentioned in this Section, see Section 16.

Classification (67/548/EEC or 1999/45/EC)

F	Highly flammable	R11
Carc.Cat.1	Carcinogenic Category 1	R45
Mut.Cat.2	Mutagenic Category 2	R46
Xi	Irritant	R36/38
T	Toxic	R48/23/24/25
Xn	Harmful	R65

For the full text of the R-phrases mentioned in this Section, see Section 16.

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2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H340 May cause genetic defects.
H350 May cause cancer.
H225 Highly flammable liquid and vapour.
H304 May be fatal if swallowed and enters airways.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H372 Causes damage to organs through prolonged or repeated exposure.

Precautionary statements

Prevention

P201 Obtain special instructions before use.
P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P240 Ground/bond container and receiving equipment.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P314 Get medical advice/ attention if you feel unwell.

Storage

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

General hazard statement not specifying the route of exposure as the necessary information is not available. See Annex VI, 1.2.2, Note is not defined in the proposal.

Restricted to professional users.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H304 May be fatal if swallowed and enters airways.
H340 May cause genetic defects.
H350 May cause cancer.
H372 Causes damage to organs through prolonged or repeated exposure.

Precautionary statements

P201 Obtain special instructions before use.

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P314 Get medical advice/ attention if you feel unwell.

CAS-No. 1076-43-3

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula C₆D₆ (Hill)
EC-No. 214-061-8
Molar mass 84,15 g/mol

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
(2H6)benzene (<= 100 %)		
1076-43-3	*)	Flammable liquid, Category 2, H225 Carcinogenicity, Category 1A, H350 Germ cell mutagenicity, Category 1B, H340 Specific target organ toxicity - repeated exposure, Category 1, H372 Aspiration hazard, Category 1, H304 Eye irritation, Category 2, H319 Skin irritation, Category 2, H315

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

For the full text of the H-Statements mentioned in this Section, see Section 16.

Hazardous components (1999/45/EC)

Chemical Name (Concentration)

CAS-No.	Classification
(2H6)benzene (<= 100 %)	
1076-43-3	F, Highly flammable; R11 Carc.Cat.1; R45 Mut.Cat.2; R46 Xi, Irritant; R36/38 T, Toxic; R48/23/24/25 Xn, Harmful; R65

For the full text of the R-phrases mentioned in this Section, see Section 16.

3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

General advice

First aider needs to protect himself.

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After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Consult a physician.

After eye contact: rinse out with plenty of water. Call in ophthalmologist.

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Call a physician immediately. Pulmonary failure possible after aspiration of vomit.

4.2 Most important symptoms and effects, both acute and delayed

irritant effects

Dizziness, narcosis, inebriation, euphoria, agitation, Headache, Tiredness, CNS disorders, respiratory arrest, Nausea

Repeated exposure may cause skin dryness or cracking.

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam, Carbon dioxide (CO₂), Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Combustible.

Pay attention to flashback.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air at ambient temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Special protective equipment for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

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6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorised persons.

Recommended storage temperature see product label.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material: Viton (R)

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splash contact:	Glove thickness:	0,70 mm
	Break through time:	> 480 min
	Glove material:	Nitrile rubber
	Glove thickness:	0,40 mm
	Break through time:	> 10 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 890 Vitoject® (full contact), KCL 730 Camatril® -Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter A-(P3)

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not let product enter drains.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	aromatic
Odour Threshold	5 ppm
pH	No information available.
Melting point	6,7 °C
Boiling point/boiling range	79 °C at 1.013 hPa
Flash point	-11 °C Method: DIN 51755 Part 1
Evaporation rate	No information available.

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Flammability (solid, gas)	Not applicable
Lower explosion limit	1,4 %(V)
Upper explosion limit	8,0 %(V)
Vapour pressure	101 hPa at 20 °C
Relative vapour density	2,7
Density	0,95 g/cm3 at 20 °C
Relative density	No information available.
Water solubility	1,8 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 2,13 (experimental) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

Ignition temperature	555 °C Method: DIN 51794
Viscosity, kinematic	0,78 mm2/s at 20 °C

SECTION 10. Stability and reactivity

10.1 Reactivity

steam-volatile

Vapours may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Exothermic reaction with:

halogens, uranium hexafluoride

Halogenated hydrocarbon, in the presence of:

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Light metals

Risk of explosion with:

halogen-halogen compounds, Nitric acid, Ozone, peroxi compounds, perchlorates, permanganic acid, perchloryl fluoride, Strong oxidizing agents, Chlorine, fluorides

Risk of ignition or formation of inflammable gases or vapours with:

chromium(VI) oxide, Fluorine, nitril compounds, Oxygen, oxyhalogenic compounds

Violent reactions possible with:

mineral acids, sulfur

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

rubber, various plastics

10.6 Hazardous decomposition products

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

Symptoms: Nausea
absorption

Acute inhalation toxicity

LC50 Rat: 44 mg/l; 4 h ; vapour
(IUCLID)

Symptoms: Possible damages:, mucosal irritations

Acute dermal toxicity

LD50 Rabbit: > 8.260 mg/kg
(IUCLID)

absorption

Skin irritation

Rabbit

Result: Irritations

OECD Test Guideline 404

Causes skin irritation.

Drying-out effect resulting in rough and chapped skin.

Eye irritation

Rabbit

Result: Eye irritation

(IUCLID)

Causes serious eye irritation.

Sensitisation

This information is not available.

Germ cell mutagenicity

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Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

(National Toxicology Program)

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

CMR effects

Carcinogenicity:

May cause cancer. Positive evidence from human epidemiological studies.

Mutagenicity:

May cause genetic defects.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

Causes damage to organs through prolonged or repeated exposure.

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary oedema and pneumonitis.

11.2 Further information

Systemic effects:

After absorption:

agitation, euphoria, Headache, Dizziness, inebriation, Tiredness, CNS disorders, narcosis, respiratory arrest

After a latency period:

Changes in the blood count, haemolysis

Further data:

This substance should be handled with particular care.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 *S.gairdnerii*: 5,9 mg/l; 96 h

OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

EC50 *Daphnia magna* (Water flea): 9,2 mg/l; 48 h

(ECOTOX Database)

Toxicity to algae

IC50 *Pseudokirchneriella subcapitata* (green algae): 29 mg/l; 72 h

OECD Test Guideline 201

Toxicity to bacteria

EC10 *Pseudomonas putida*: 168 mg/l

(Lit.)

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12.2 Persistence and degradability

Biodegradability

Readily biodegradable

Theoretical oxygen demand (ThOD)

3.100 mg/g

(Lit.)

Ratio BOD/ThBOD

BOD5 71 %

(Lit.)

Ratio COD/ThBOD

19 %

(Lit.)

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2,13

(experimental)

(Lit.) Bioaccumulation is not expected.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Henry constant

562 Pa·m³/mol

at 25 °C

Method: (calculated)

(Lit.) Distribution preferentially in air.

Additional ecological information

Biological effects:

Endangers drinking-water supplies if allowed to enter soil or water.

Discharge into the environment must be avoided.

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SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number	UN 1114
14.2 Proper shipping name	BENZENE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 1114
14.2 Proper shipping name	BENZENE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

Sea transport (IMDG)

14.1 UN number	UN 1114
14.2 Proper shipping name	BENZENE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
EmS	F-E S-D

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

SECTION 15. Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulations

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Major Accident Hazard Legislation	SEVESO III FLAMMABLE LIQUIDS P5c Quantity 1: 5.000 t Quantity 2: 50.000 t
Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.
Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC	not regulated
Substances of very high concern (SVHC)	This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).
<i>National legislation</i>	
Storage class	3

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

Details in analogy to the undeuterated compound.

Full text of H-Statements referred to under sections 2 and 3.

H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H340	May cause genetic defects.
H350	May cause cancer.
H372	Causes damage to organs through prolonged or repeated exposure.

Full text of R-phrases referred to under sections 2 and 3

R11	Highly flammable.
R36/38	Irritating to eyes and skin.
R45	May cause cancer.
R46	May cause heritable genetic damage.
R48/23/24/25	Toxic: danger of serious damage to health by prolonged exposure through inhalation, in contact with skin and if swallowed.
R65	Harmful: may cause lung damage if swallowed.

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Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

Hazard statements

H225 Highly flammable liquid and vapour.
H304 May be fatal if swallowed and enters airways.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
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Precautionary statements

Prevention

P201 Obtain special instructions before use.
P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P240 Ground/bond container and receiving equipment.

Response



P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P314 Get medical advice/ attention if you feel unwell.

Storage

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

Restricted to professional users.

Labelling (67/548/EEC or 1999/45/EC)

<i>Symbol(s)</i>	 F  T	Highly flammable Toxic
<i>R-phrases(s)</i>	45-46-48/23/24/25- 65-11-36/38	May cause cancer. May cause heritable genetic damage. Also toxic: danger of serious damage to health by prolonged exposure through inhalation, in contact with skin and if swallowed. Also harmful: may cause lung damage if swallowed. Highly flammable. Irritating to eyes and skin.
<i>S-phrases(s)</i>	53-45	Avoid exposure - obtain special instructions before use. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

Further information



Restricted to professional users. Only for research, development, analysis or specific industrial processes (76/769/EEC).

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Reduced labelling (≤125 ml)

Symbol(s)   F
T

R-phrases 45-46-48/23/24/25-65

S-phrases 53-45

Highly flammable
Toxic

May cause cancer. May cause heritable genetic damage. Also toxic: danger of serious damage to health by prolonged exposure through inhalation, in contact with skin and if swallowed. Also harmful: may cause lung damage if swallowed.
Avoid exposure - obtain special instructions before use. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.